Laboratoire de Biochimie Théorique
Institut de **B**iologie **P**hysico-**C**himique
13, rue Pierre et Marie Curie
75005 PARIS

S E M I N A I R E

Fabio Pietrucci

Sorbonne Université, IMPMC, Paris

« Free energy landscapes and kinetics of protein folding and association »

Predicting detailed structural, thermodynamic and kinetic properties of biomolecular processes starting from atomistic simulations is a long-standing computational challenge. Several enhanced sampling techniques can be applied with reasonable confidence to reconstruct free energy landscapes, whereas the access to kinetic predictions is hampered by more theoretical and practical hurdles. I will discuss advantages and limitations of a few tools we developed in the last years, with applications to globular and intrinsically disordered proteins as well as to protein-protein interaction. In particular, I will focus on the two main classes of kinetic tools: Markov state models and Langevin models. In the first case, the dynamics of the system is coarse-grained into memory-less jumps among a discrete set of conformational states. In the second case, the dynamics projected onto a few collective variables is approximated with a stochastic differential equation, possibly non-Markovian. In both cases, I will present ideas allowing to circumvent the time-scale problem, i.e. the problem of generating extremely long ergodic trajectories reversibly sampling the transitions between metastable states.

[1] C. Camilloni and F. Pietrucci, Adv. Phys. X 3, 1477531 (2018)
[2] F. Pietrucci, Rev. Phys. 2, 32 (2017)
[3] F. Pietrucci, A.V. Vargiu, A. Kranjc, Sci. Rep. 5, 18555 (2015)
[4] A. Pérez-Villa and F. Pietrucci, arXiv 1810.00713 (2018)

Mercredi 27 novembre 2019
09h45

SALLE DE CONFERENCE